

Joint Research Centre

webKORIGEN: Web-based Nuclide Depletion Calculations

presented by Jozsef Zsigrai

www.jrc.ec.europa.eu

*Serving society
Stimulating innovation
Supporting legislation*



webKORIGEN history

- ORIGEN: Oak Ridge Isotope Generation and Depletion Code
- ORIGEN2: A Revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code
- KORIGEN: Karlsruhe ORIGEN, optimized for German reactors
- webKORIGEN: Version of KORIGEN driven by the EU-web-portal Nucleonica, with a subset of KORIGEN features

Purpose:

- Calculate fuel nuclide inventory changed by neutron interactions and decays

webKORIGEN fields of application:

- From the initial amount and composition of a nuclear fuel and a given irradiation history it determines the fuel nuclide inventory changed by neutron interactions and decays
- Initial actinides daughters and FP are considered
- n-interactions: (n,f) , (n,γ) , $(n,2n)$, $(n,3n)$
- Decays: α , β^- , β^+ , internal transitions
- Calculated Quantities for Nuclides and Chemical Elements:
 - Concentrations (mol or g)
 - Radioactivities (Bq)
 - Total and γ -heat releases (W)
 - Radiotoxicities for ingestion and inhalation (Sv)
 - Gamma and neutron emission rates (γ/s , n/s)

webKORIGEN features:

- Follow-up of nuclide generation in a neutron field (reactor, irradiation facility) and during subsequent decay, including re-processing
- Easy-to-use Graphical User Interface:
menus, toolbars, online help
- Easy input preparation restricted to simple basic applications
- A subset of full KORIGEN features, dedicated data libraries
- Fast graphical output generation



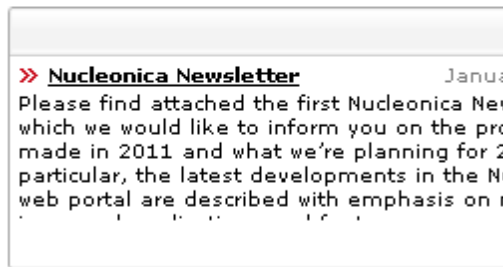
The screenshot shows the Nucleonica web application interface. At the top, there is a blue header with the Nucleonica logo and the tagline "... web driven nuclear". Below the header is a navigation bar with tabs: Applications, Data, Knowledge, My Preferences, Print, Networking, Nuclear Science, and Home. The Applications tab is selected, and a dropdown menu is displayed. The menu lists various applications: Nuclide Explorer, Mass Activity Calculator, Mass Activity Converter, Decay Engine, Dosimetry and Shielding, Range and Stopping Power, In Silico Dosimetry, **webKORIGEN** (highlighted with a red rectangle), Decay Engine for Large Nuclide Sets, Universal Nuclide Chart, Transport and Packaging, Nuclide Mixtures, Nucleonica Scripting, Gamma Spectrum Generator, Gamma Spectrum Generator Pro, Virtual Cloud Chamber, Cambio file converter, WESPA, Gamma Library, and webGraph.

Accessing webKORIGEN

1. Select Applications->webKORIGEN from the Nucleonica's main menu

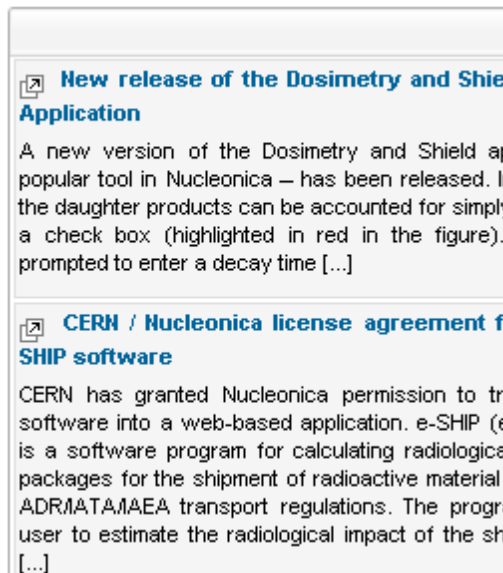
OR

2. Go to the Nuclear Science Applications Portal and select webKORIGEN from the application list



>> Nucleonica Newsletter January
Please find attached the first Nucleonica Newsletter which we would like to inform you on the products made in 2011 and what we're planning for 2012. In particular, the latest developments in the Nucleonica web portal are described with emphasis on the new features.

>> Nucleonica Blog



New release of the Dosimetry and Shielding Application
A new version of the Dosimetry and Shielding Application, a popular tool in Nucleonica – has been released. In this version, the daughter products can be accounted for simply by checking a checkbox (highlighted in red in the figure), which prompts the user to enter a decay time [...]

CERN / Nucleonica license agreement for e-SHIP software
CERN has granted Nucleonica permission to transform the e-SHIP software into a web-based application. e-SHIP (e-SHIP) is a software program for calculating radiological impact packages for the shipment of radioactive material according to ADR/MATA/IAEA transport regulations. The program allows the user to estimate the radiological impact of the shipment [...]



webKORIGEN

[Questions, remarks, suggestions can be posted in the forum](#)

webKORIGEN was developed from the Oak Ridge Isotope Generation and Depletion code ORIGEN. Starting with a given initial reactor fuel or a single target nuclide, it calculates the time evolution of nuclide densities changing due to decays and neutron-induced reactions, and determines derived nuclear properties such as masses, radioactivities, heat releases, radiotoxicities, emission of radiation, etc...

Step 1: Calculation Mode

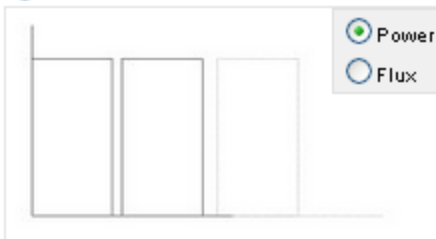
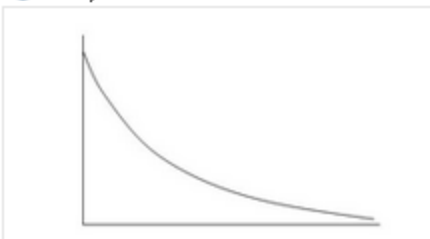
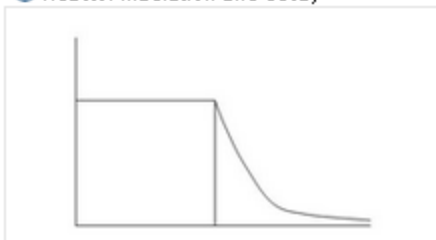
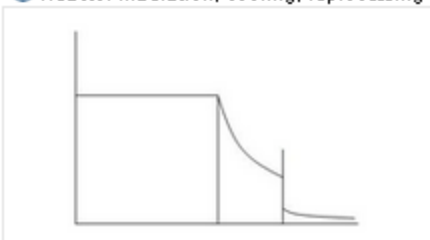
Step 2: Reactor / Operation

Step 3: Input Summary and Run

Step 4: Display Results

Step 5: Log files

Step 6: Parameters

☒ Reactor irradiation☐ Decay☐ Reactor irradiation and decay☐ Reactor irradiation, cooling, reprocessing and decay of waste

webKORIGEN calculations step by step

STEP 1: Selecting the computation mode

STEP 2: Set up of mode-dependent input parameters

STEP 3: Display of input summary and start of the execution

STEP 4: Display results

webKORIGEN calculations step by step

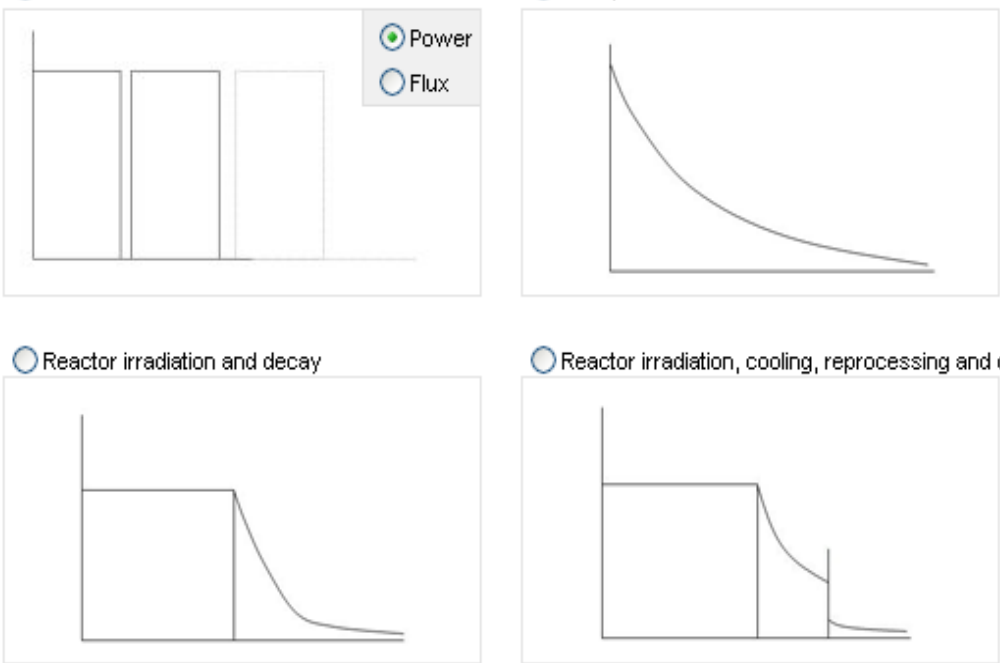
STEP 1: selecting the computation mode

Step 1: Calculation Mode Step 2: Reactor / Operation Step 3: Input Summary and Run Step 4: Display Results Step 5: Log files Step 6: Parameters

☒ Reactor irradiation ☐ Decay

☒ Power ☐ Flux

☐ Reactor irradiation and decay ☐ Reactor irradiation, cooling, reprocessing and decay of waste



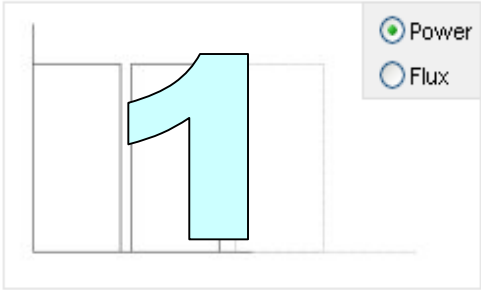
Each mode requires a different method of calculation and a different input parameter set up

webKORIGEN calculations step by step

STEP 1: selecting the computation mode

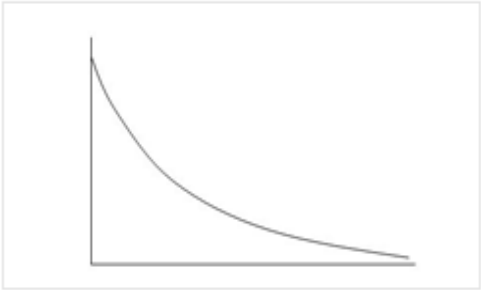
Step 1: Calculation Mode Step 2: Reactor / Operation Step 3: Input Summary and Run Step 4: Display Results Step 5: Log files Step 6: Parameters

☒ Reactor irradiation

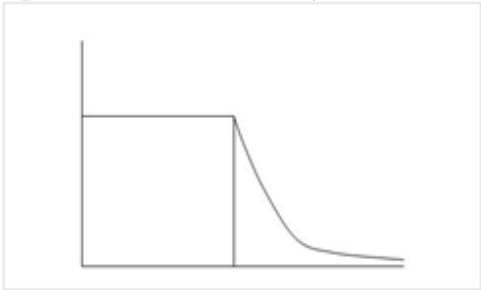


☒ Power
☐ Flux

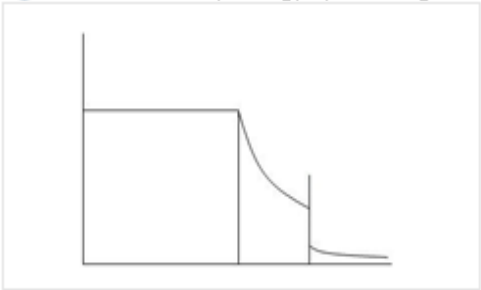
☐ Decay



☐ Reactor irradiation and decay



☐ Reactor irradiation, cooling, reprocessing and decay of waste



Mode 1:
Irradiation of fresh nuclear fuel ("Power") or of a target* ("Flux")

*Calculations of target irradiations are restricted to small samples of a single-nuclide material in larger facilities

webKORIGEN calculations step by step

STEP 1: selecting the computation mode

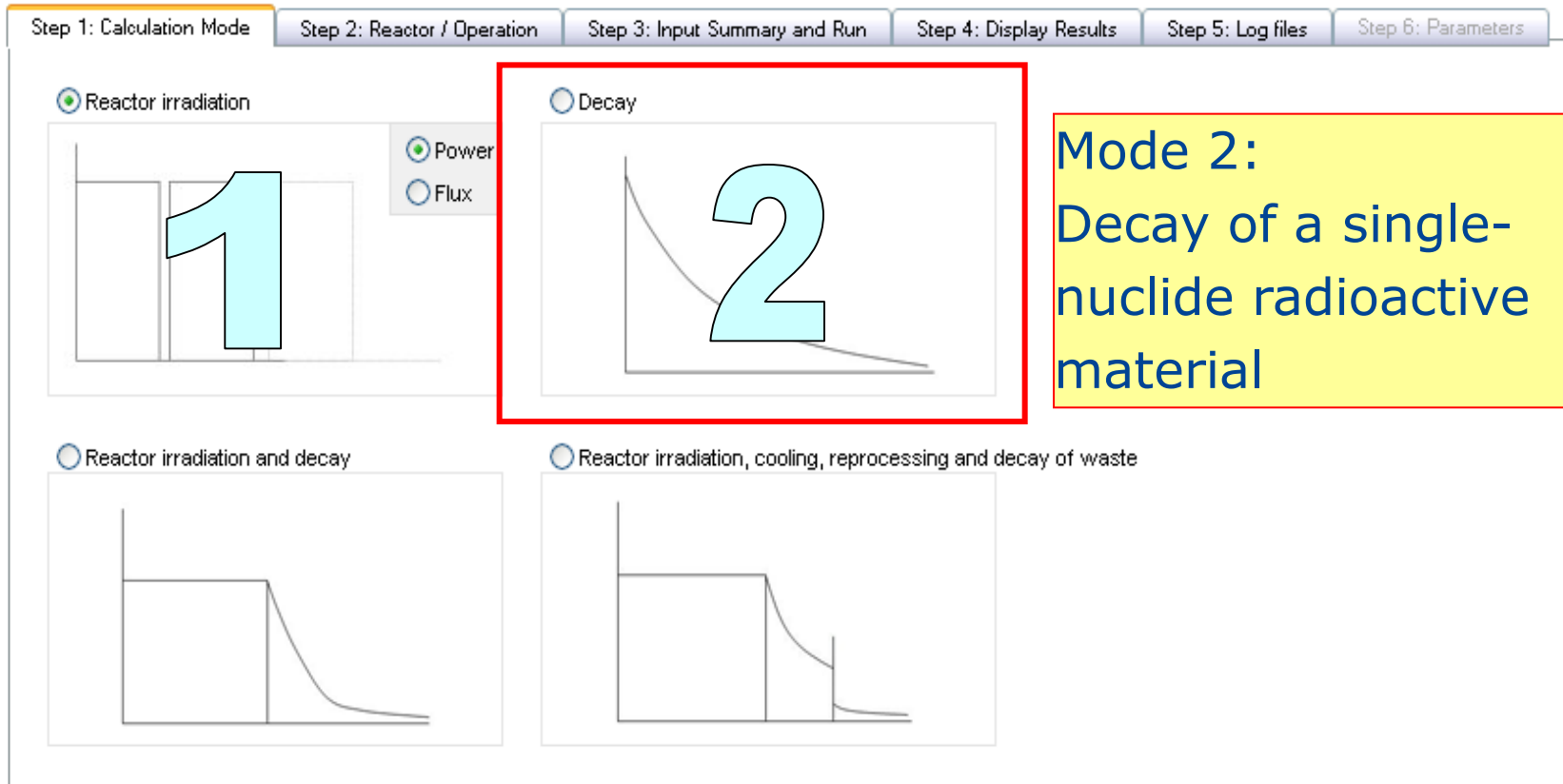
Step 1: Calculation Mode Step 2: Reactor / Operation Step 3: Input Summary and Run Step 4: Display Results Step 5: Log files Step 6: Parameters

☒ Reactor irradiation ☐ Decay

☒ Power ☐ Flux

☐ Reactor irradiation and decay ☐ Reactor irradiation, cooling, reprocessing and decay of waste

Mode 2:
Decay of a single-nuclide radioactive material



webKORIGEN calculations step by step

STEP 1: selecting the computation mode

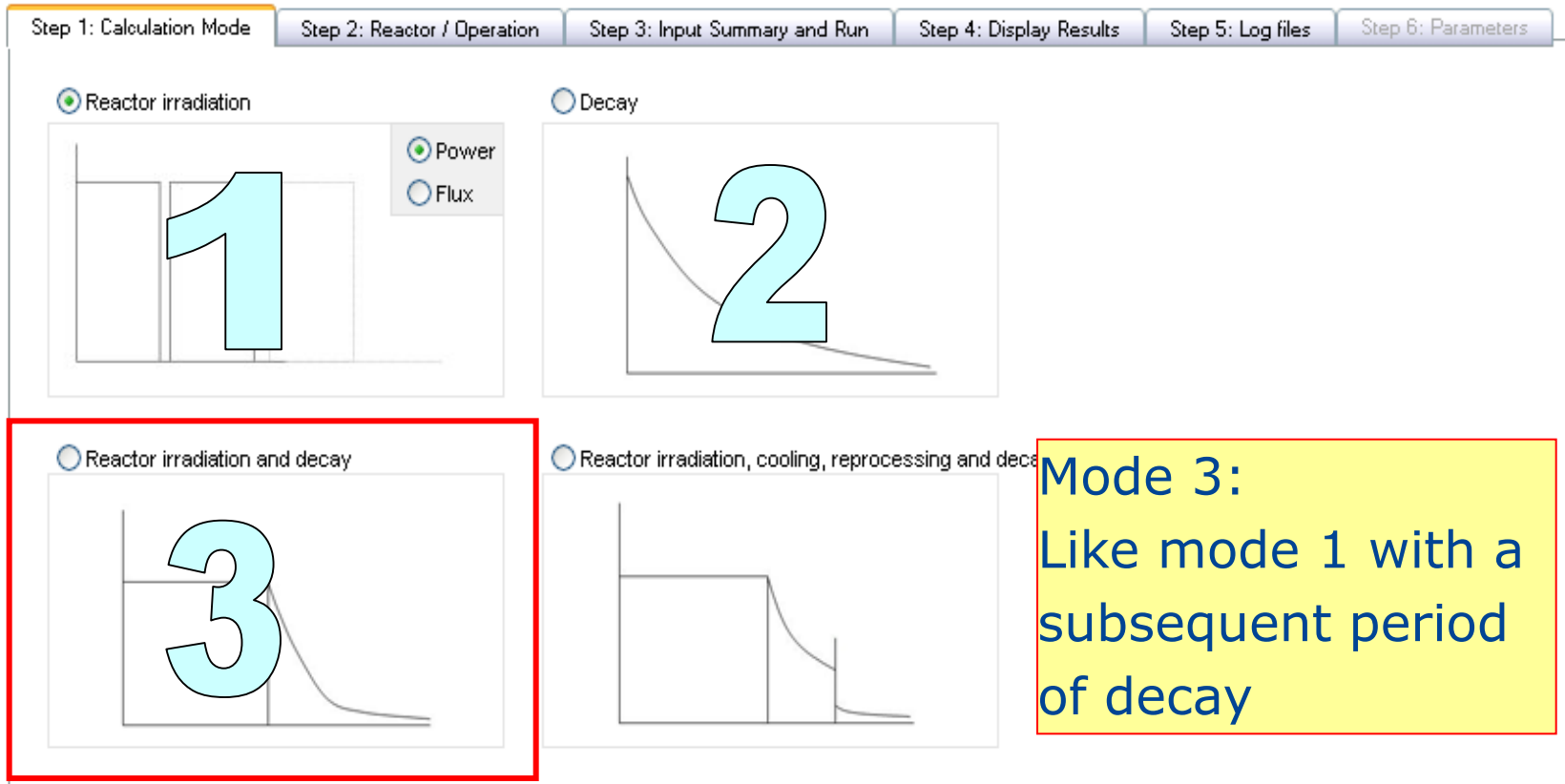
Step 1: Calculation Mode Step 2: Reactor / Operation Step 3: Input Summary and Run Step 4: Display Results Step 5: Log files Step 6: Parameters

☒ Reactor irradiation ☐ Decay

☒ Power ☐ Flux

☐ Reactor irradiation and decay ☐ Reactor irradiation, cooling, reprocessing and decay

Mode 3:
Like mode 1 with a subsequent period of decay



webKORIGEN calculations step by step

STEP 1: selecting the computation mode

Step 1: Calculation Mode Step 2: Reactor / Operation Step 3: Input Summary and Run Step 4: Display Results Step 5: Log files Step 6: Parameters

☒ Reactor irradiation ☐ Decay

☒ Power ☐ Flux

☐ Reactor irradiation and decay ☐ Reactor irradiation, cooling, reprocessing and decay of waste

Mode 4:
Like mode 3 with subsequent reprocessing and decay of waste

webKORIGEN calculations step by step

STEP 2 : set up of mode-dependent input parameters

Modes 1, 3 and 4 start with an irradiation phase, for which the reactor type, the fuel type, and the irradiation history have to be set up.

Reactor types supported by webKORIGEN:

- Thermal power plants
 - Pressurized Water Reactors (PWR)
 - Boiling Water Reactors (BWR)
 - European Fast Reactor (EFR) - a future extension to the current industrial technology

webKORIGEN calculations step by step

STEP 2 : set up of input parameters for mode 1 – an example

Step 1: Calculation Mode
Step 2: Reactor / Operation
Step 3: Input Summary and Run
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Reactor type

☒ PWR

☐ BWR

☐ EFR

Reactor Parameters

Burnup ($\text{MW}_{\text{th}} \cdot \text{d} / \text{kg}_{\text{IHM}}$):

55

Total initial heavy metal mass (t_{IHM}):

20

Electrical efficiency (%):

34

Derived Power values

Specific Power: $37.65 \text{ MW} / \text{t}_{\text{IHM}}$

Thermal Power: 0.75 GW

Electrical Power: 0.26 GW

Update power values

Initial Fuel and Neutron Spectrum

☒ UOX

U235/U (w/o) 4.0

☐ MOX

Nuclide	Weight (%)
Pu238/Pu (w/o)	2.8
Pu239/Pu (w/o)	50.5
Pu240/Pu (w/o)	27.8
Pu241/Pu (w/o)	11.5
Pu242/Pu (w/o)	7.6
Am241/Pu (w/o)	1.0

Uranium matrix

☒ Natural

☐ Depleted

Pu_{fiss}/(U+Pu) (w/o) 3.8

Irradiation and decay parameters

No. of cycles 5

Length of cycle 1 y

Load factor (%) 80.0

Cooling time before reprocessing: 6 y

Decay time after reprocessing: 100000 y

Reprocessing ratio (%)

Uranium 99.9

Plutonium 99.9

Neptunium 99.5

Americium 99.5

Curium 99.5

webKORIGEN calculations step by step

STEP 3 : Display of input summary and start of the execution

Step 1: Calculation Mode Step 2: Reactor / Operation **Step 3: Input Summary and Run** Step 4: Display Results Step 5: Log files Step 6: Parameters

Input summary

Mode of calculation:	Reactor irradiation in power mode
Burnup:	55 MWd/kg
Reactor type:	PWR
Fuel:	UOX with 4.0% enrichment
Cross Section Library:	<input checked="" type="radio"/> PWR UOX 4.0% U235 60MWd/kgHM <input type="radio"/> PWR UOX high burnup (ORNL)
Operation parameters:	<div>No. of cycles: 5 Length of cycle: 1 y Load factor: 80.0 % Heavy metal mass: 20 t</div>

Run calculation

Run calculation

webKORIGEN calculations step by step

STEP 4: Display results – example: output in tables

Step 1: Calculation Mode Step 2: Reactor / Operation Step 3: Input Summary and Run **Step 4: Display Results** Step 5: Log files Step 6: Parameters

Display results for nuclides/elements dominant at 4.8 y irradiation

Nuclides/Elements Radiations Nuclide Chart

Display quantity: **Mass (g)** Filter: Save as Mixture ...of up to 20 selected Nuclides

Plot	Z	Nuclides	Results	Plot	Z	Elements	Results	Plots	Totals	Nuclides	Elements	Results
<input type="checkbox"/>	92	U238	1.841e+7	<input type="checkbox"/>	92	Uranium	1.861e+7	<input type="checkbox"/>	Actinides+Progenies:	101	19	1.887e+7
<input type="checkbox"/>	94	Pu239	1.107e+5	<input type="checkbox"/>	94	Plutonium	2.335e+5	<input type="checkbox"/>	Actinides:	65	11	1.887e+7
<input type="checkbox"/>	92	U236	1.090e+5	<input type="checkbox"/>	54	Xenon	1.699e+5	<input type="checkbox"/>	Transuraniums:	40	7	2.612e+5

<input type="checkbox"/>	55	Cs133	3.391e+4	<input type="checkbox"/>	93	Neptunium	1.751e+4
<input type="checkbox"/>	42	Mo100	2.924e+4	<input type="checkbox"/>	39	Yttrium	1.428e+4
<input type="checkbox"/>	42	Mo98	2.788e+4	<input type="checkbox"/>	45	Rhodium	1.207e+4
<input type="checkbox"/>	40	Zr96	2.590e+4	<input type="checkbox"/>	36	Krypton	1.121e+4
<input type="checkbox"/>	0	963	1.997e+7	<input type="checkbox"/>	66		1.997e+7

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Download ☒ Excel ☐ CSV Comma (",") ☐ Use field qualifier ("") ☒ Nuclides ☐ Elements

Plot Nuclides Plot Elements Plot Totals Plot Element Distribution

Quantity to be displayed

- Mass (mole or gram)
- Activity (Bq)
- Decay heat (W)
- Gamma emission rate (W)
- Radiotoxicities (Sv)

webKORIGEN calculations step by step

STEP 4: Display results – example: output in graphs

Step 1: Calculation Mode Step 2: Reactor / Operation Step 3: Input Summary and Run **Step 4: Display Results** Step 5: Log files Step 6: Parameters

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Download Excel CSV Comma (",") Use field qualifier (") Nuclides Elements

2 significant figures

Plot Nuclides Plot Elements Plot Totals Plot Element Distribution

Plot

- Nuclides
- Elements
- Totals
- Element distribution

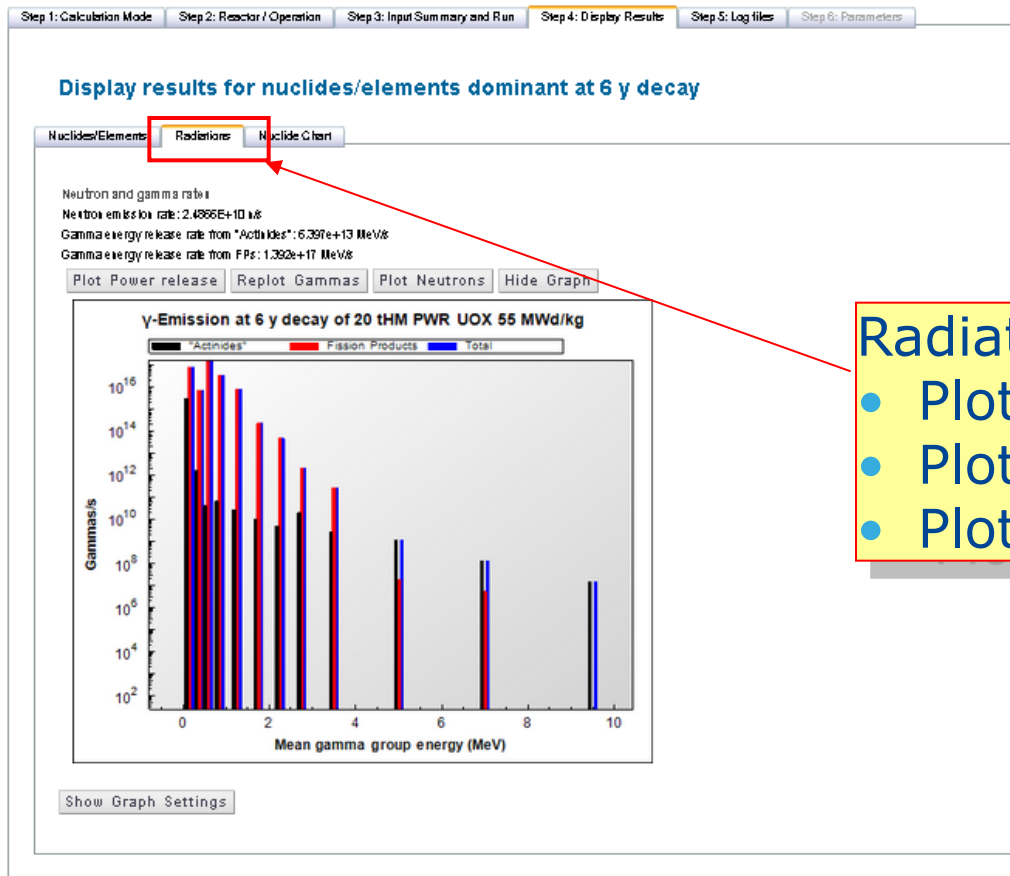
webKORIGEN calculations step by step

STEP 4: Display results – example: output in graphs



webKORIGEN calculations step by step

STEP 4: Display results – example: output in graphs

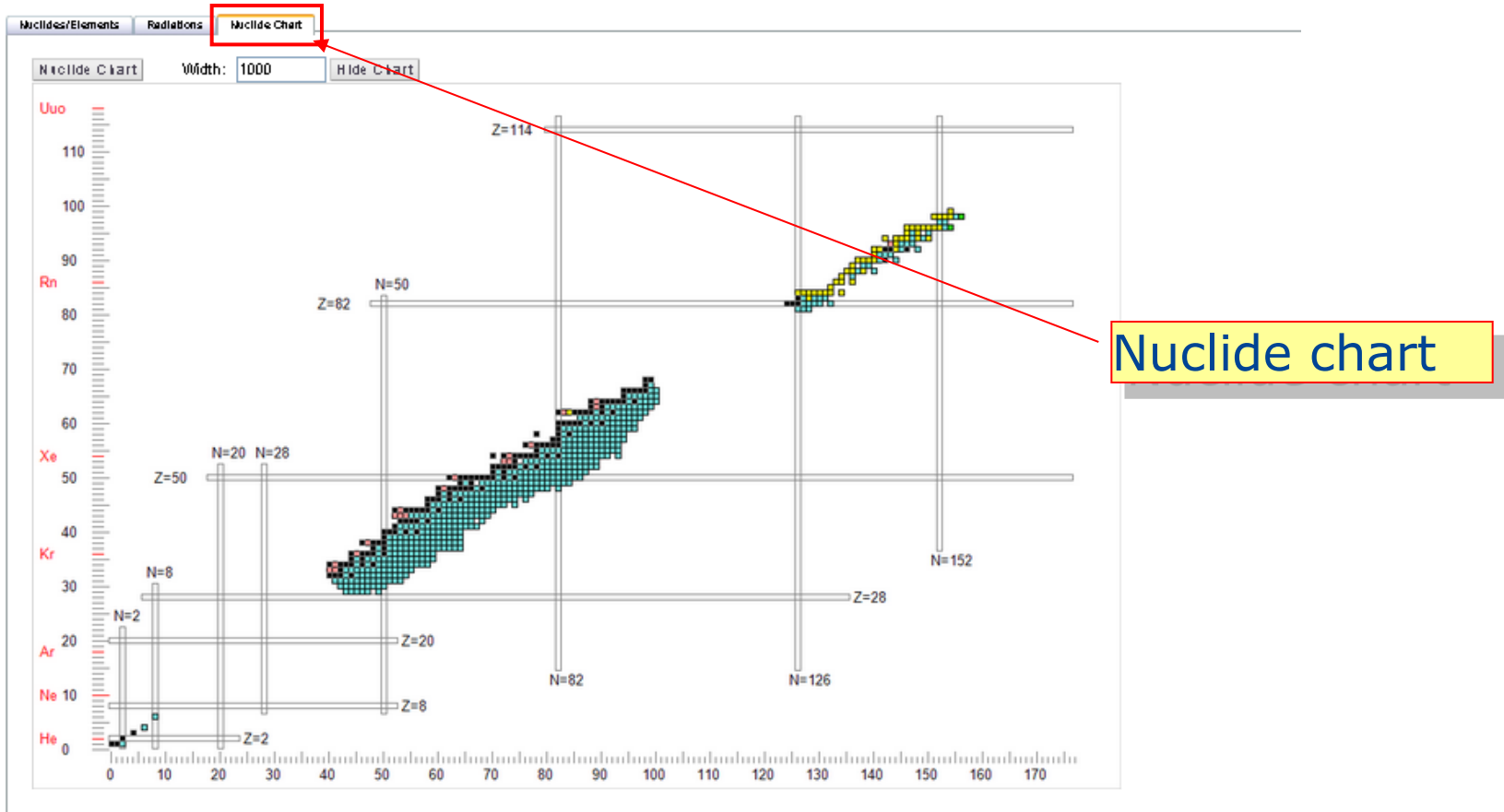


Radiations

- Plot power release
- Plot gammas
- Plot neutrons

webKORIGEN calculations step by step

STEP 4: Display results – example: output in graphs



webKORIGEN calculations step by step

STEP 4: Display results – example

Step 1: Calculation Mode Step 2: Reactor / Operation Step 3: Input Summary and Run **Step 4: Display Results** Step 5: Log files Step 6: Parameters

Display results for nuclides/elements dominant at 4.8 y irradiation

Nuclides/Elements Radiations Nuclide Chart

Display quantity: Filter:

...of up to 20 selected Nuclides

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Download ☒ Excel ☐ CSV Comma (",") ☐ Use field qualifier ("") ☒ Nuclides ☐ Elements 2 significant figures

Save selected nuclides as mixture

Exercise 1

Following the irradiation of UO_2 fuel in a PWR and 30 years cooling, calculate the activities of Cs137 and Sr90 fission products (show a graph of activities over the 30 y period)

1. Calculation mode: "Reactor irradiation and decay"
2. Reactor operation:
 - Reactor type: PWR
 - Fuel: UOX with default enrichment (4.0 %)
 - Irradiation and decay parameters:
 - Fuel decay time after discharge: 30 years
 - default values for burn-up, number of cycles etc.
3. Run calculation
4. Examine results: Display quantity: Activity (Bq)
5. Select Cs137 and Sr90 in the table
6. Plot nuclides

Exercise 2

Calculate the fission yield of Ba139 from the irradiation of 1g U235 (from enriched uranium) in a thermal neutron spectrum (flux $7 \times 10^{11} \text{ cm}^2\text{s}^{-1}$) during 30 minutes (show a graph of the mass of Ba139 produced during the 30 minute irradiation).

1. Calculation mode: "Reactor irradiation (Flux)"
 - Flux = 7×10^{11}
2. Reactor operation:
 - Reactor type: PWR
 - Fuel: UOX with default enrichment (4.0 %)
 - Single nuclide irradiation: U235
 - Initial mass: 1g
 - Irradiation time: 3 min
3. Run calculation
4. Examine results: Display quantity: Mass (g)
5. Select Ba139
6. Plot nuclides

Exercise 3

Dose rate from spent fuel after 6 years cooling

1. Set up a “Reactor irradiation and decay” calculation for a PWR reactor with UOX, using default values for burn-up, fuel enrichment, number of cycles etc.
2. Run calculation
3. Examine results
4. Select the top 20 nuclides with highest gamma emission rates and save them as a nuclide mixture
5. Go to the *Dosimetry and shielding* application
6. In the mixture selector select “webKorigen nuclides”
 - Include daughters!
7. Do a dose rate calculation as usual